

FILE 'HOME' ENTERED AT 15:58:45 ON 26 JAN 2007

=> file registry

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 15:59:02 ON 26 JAN 2007

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STRUCTURE FILE UPDATES: 25 JAN 2007 HIGHEST RN 918475-45-3

DICTIONARY FILE UPDATES: 25 JAN 2007 HIGHEST RN 918475-45-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

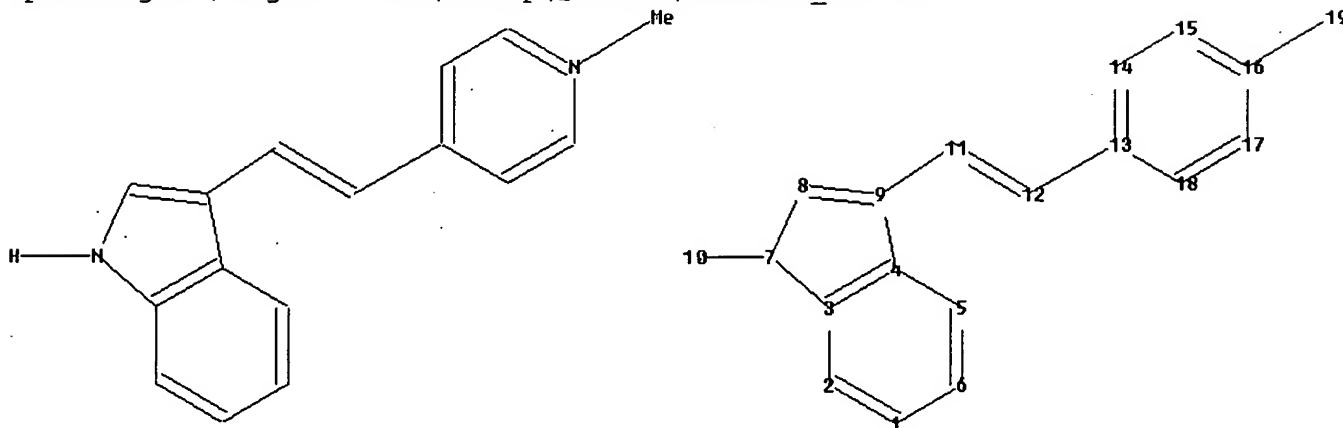
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10613762\_str.str



chain nodes :

10 11 12 19

ring nodes :

1 2 3 4 5 6 7 8 9 13 14 15 16 17 18

chain bonds :

7-10 9-11 11-12 12-13 16-19

ring bonds :

1-2 1-6 2-3 3-4 3-7 4-5 4-9 5-6 7-8 8-9 13-14 13-18 14-15 15-16 16-17 17-18

exact/norm bonds :

3-7 4-9 7-8 8-9

exact bonds :

7-10 9-11 11-12 12-13 16-19

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS

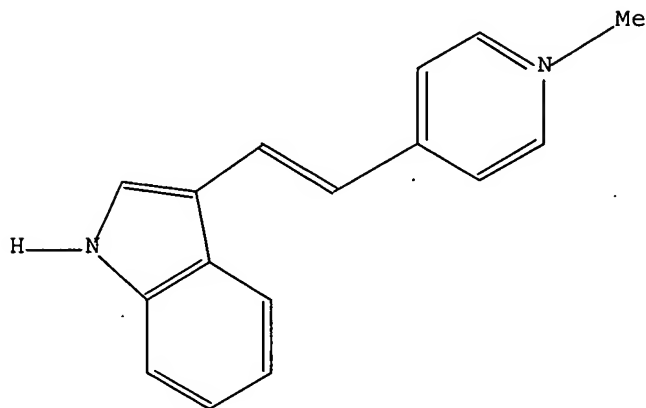
11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 15:59:20 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 50 TO ITERATE

100.0% PROCESSED 50 ITERATIONS

2 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 576 TO 1424

PROJECTED ANSWERS: 2 TO 124

L2 2 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 15:59:24 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 905 TO ITERATE

100.0% PROCESSED 905 ITERATIONS

27 ANSWERS

SEARCH TIME: 00.00.01

L3 27 SEA SSS FUL L1

=> file medline, caplus, wpids, uspatfull

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

172.10

172.31

FILE 'MEDLINE' ENTERED AT 15:59:33 ON 26 JAN 2007

FILE 'CAPLUS' ENTERED AT 15:59:33 ON 26 JAN 2007

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FILE 'WPIDS' ENTERED AT 15:59:33 ON 26 JAN 2007

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FILE 'USPATFULL' ENTERED AT 15:59:33 ON 26 JAN 2007

CA INDEXING COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

=> s 13

SAMPLE SEARCH INITIATED 15:59:38 FILE 'WPIDS'

SAMPLE SCREEN SEARCH COMPLETED - 1 TO ITERATE

100.0% PROCESSED

1 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 1 TO 40

PROJECTED ANSWERS: 0 TO 0

L4 58 L3

=> s 14 not py>2001

L5 16 L4 NOT PY>2001

=> d 15 1-16 ibib, abs, hitstr

L5 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:826093 CAPLUS Full-text

DOCUMENT NUMBER: 136:61809

TITLE: Indole- and carbazole-substituted pyridinium iodide salts: a rare case of conformational isomerism in crystals

AUTHOR(S): Wang, Zheng; Nesterov, Vladimir N.; Borbulevych, Oleg Ya.; Clark, Ronald D.; Antipin, Mikhail Yu.; Timofeeva, Tatiana V.

CORPORATE SOURCE: Department of Chemistry, New Mexico Highlands University, Las Vegas, NM, 87701, USA

SOURCE: Acta Crystallographica, Section C: Crystal Structure Communications (2001), C57(11), 1343-1348  
CODEN: ACSCEE; ISSN: 0108-2701

PUBLISHER: Munksgaard International Publishers Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Indole- and carbazole-substituted pyridinium iodide salts were synthesized and characterized. X-ray anal. revealed that the iodide salt of the indole-

substituted cation (E)-4-(1H-indol-3-ylvinyl)-N-methylpyridinium (IMPE+), C<sub>16</sub>H<sub>15</sub>N<sub>2</sub><sup>+</sup>·I<sup>-</sup>, (I), has two polymorphic modifications, (Ia) and (Ib), and a hemihydrate structure, C<sub>16</sub>H<sub>15</sub>N<sub>2</sub><sup>+</sup>·I<sup>-</sup>·0.5H<sub>2</sub>O, (II). Until now, only one crystal modification was identified for the (E)-4-(9-ethyl-9H-carbazol-3-ylvinyl)-N-methylpyridinium (ECMPE+) iodide salt, C<sub>22</sub>H<sub>21</sub>N<sub>2</sub><sup>+</sup>·I<sup>-</sup>, (III). Crystals of (Ia) and (Ib) comprise stacks of antiparallel cations with iodide anions located in the channels between the stacks. Due to the presence of the H<sub>2</sub>O mols., the packing in (II) is quite different to that found in (Ia) and (Ib), and positional disorder involving a statistical superposition of two rotamers of IMPE+, with different orientations of the indole fragment, was found. Crystals of (III) contain two independent ECMPE+ rotamers with different orientations of their carbazole substituents. The cations are packed in stacks, with the iodide anions located in the channels between the stacks. In (III), the iodide is disordered over two sites, with occupancies of 0.83 and 0.17. Crystallog. data are given.

IT 382591-35-7

RL: PRP (Properties)  
(crystal structure of)

RN 382591-35-7 CAPLUS

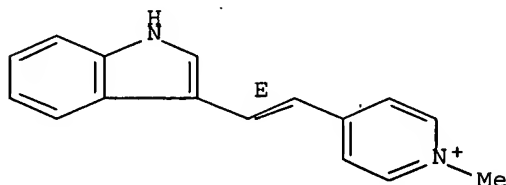
CN Pyridinium, 4-[(1E)-2-(1H-indol-3-yl)ethenyl]-1-methyl-, iodide, hydrate  
(2:1) (9CI) (CA INDEX NAME)

CM 1

CRN 36098-33-6

CMF C<sub>16</sub> H<sub>15</sub> N<sub>2</sub> . I

Double bond geometry as shown.



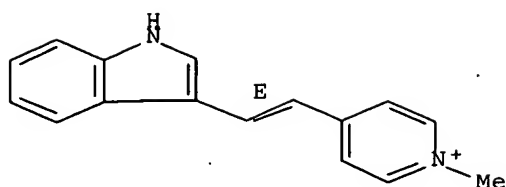
IT 36098-33-6P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and crystal structure of polymorphs of)

RN 36098-33-6 CAPLUS

CN Pyridinium, 4-[(1E)-2-(1H-indol-3-yl)ethenyl]-1-methyl-, iodide (9CI) (CA INDEX NAME)

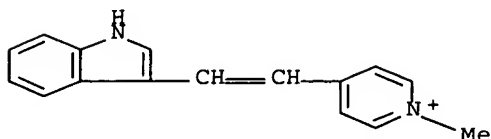
Double bond geometry as shown.



● I<sup>-</sup>

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

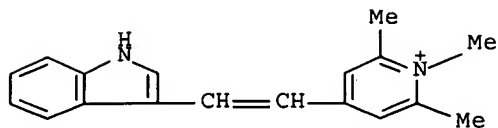
L5 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN ?  
 ACCESSION NUMBER: 1999:332021 CAPLUS Full-text ?  
 DOCUMENT NUMBER: 131:96967  
 TITLE: Substituted 2- and 4-[2-(3-indolyl)ethenyl]pyridinium salts as inhibitors of MAO-B. Quantitative modeling of the structure-activity relationship  
 AUTHOR(S): Bachurin, S. O.; Fetison, V. I.; Afanas'ev, A. Z.; Afanas'eva, S. V.; Dubova, L. G.; Yankovskaya, V. L.; Mukhina, T. V.  
 CORPORATE SOURCE: Inst. Fiziol. Aktivnykh Veshchestv, Ross. Akad. Nauk, Chernogolovka, Russia  
 SOURCE: Doklady Akademii Nauk (1999), 364(6), 782-785  
 CODEN: DAKNEQ; ISSN: 0869-5652  
 PUBLISHER: MAIK Nauka  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 AB Synthesis of 21 monoamineoxidase B inhibitors is reported. The modeling data demonstrate that combination of hydrophobic, polar, and steric factors det. the degree of the enzyme inhibition.  
 IT 26608-75-3P 231954-87-3P 231955-03-6P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
 (substituted 2- and 4-[2-(3-indolyl)ethenyl]pyridinium salts as inhibitors of MAO-B: structure-activity relationship)  
 RN 26608-75-3 CAPLUS  
 CN Pyridinium, 4-[2-(1H-indol-3-yl)ethenyl]-1-methyl-, iodide (9CI) (CA INDEX NAME)



● I<sup>-</sup>

RN 231954-87-3 CAPLUS

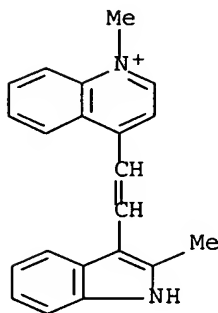
CN Pyridinium, 4-[2-(1H-indol-3-yl)ethenyl]-1,2,6-trimethyl-, iodide (9CI)  
(CA INDEX NAME)



● I<sup>-</sup>

RN 231955-03-6 CAPLUS

CN Quinolinium, 1-methyl-4-[2-(2-methyl-1H-indol-3-yl)ethenyl]-, iodide (9CI)  
(CA INDEX NAME)



● I<sup>-</sup>

L5 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1996:434896 CAPLUS Full-text ?

DOCUMENT NUMBER: 125:54703

TITLE: Inhibition of dopamine reuptake system by analog of neurotoxic metabolite MPP(1-methyl-4-phenylpyridinium). Structure-activity relationships

AUTHOR(S): Bachurin, S. O.; Lukoyanov, N. V.; Petrova, L. N.; Solyakov, L. S.; Tkachenko, S. E.; Raevskii, O. A.

CORPORATE SOURCE: Institut Fiziologicheskii Aktivnykh Veshchestv, Chernogolovka, Russia

SOURCE: Doklady Akademii Nauk (1996), 346(4), 549-551  
CODEN: DAKNEQ; ISSN: 0869-5652

PUBLISHER: MAIK Nauka

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB The quant. structure-activity anal. (QSAR) was carried out for 41 potential inhibitors of dopamine (I) reuptake of the series of 1-methyl-4-phenyl-1,2,3,4-tetrahydropyridine, 1-methyl-4-phenylpyridine, and stilbazole analogs. The structure-activity correlation equations were developed. QSAR demonstrated that the charge on the N atom of the pyridine cycle and hydrophilic substituents enhanced the inhibiting ability of the compds., while

the substituents more electroneg. than the N atom of the pyridine cycle caused a decrease in the affinity of the compds. to a I carrier.

IT 177997-46-5

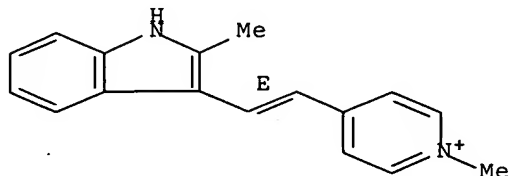
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(QSAR study of inhibition of dopamine reuptake system by methylphenylpyridine analogs)

RN 177997-46-5 CAPLUS

CN Pyridinium, 1-methyl-4-[2-(2-methyl-1H-indol-3-yl)ethenyl]-, (E)- (9CI)  
(CA INDEX NAME)

Double bond geometry as shown.



L5 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1988:159032 CAPLUS Full-text

DOCUMENT NUMBER: 108:159032

TITLE: Photolithographic material containing contrast-enhancing layer

INVENTOR(S): Ichimura, Kunihiro; Yonezawa, Teruhiko; Kikuchi, Hideo; Tochizawa, Nariaki; Hayashi, Keiichi

PATENT ASSIGNEE(S): Agency of Industrial Sciences and Technology, Japan; Toyo Gosei Kogyo Co., Ltd.

SOURCE: Eur. Pat. Appl., 31 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 246885	A2	19871125	EP 1987-304498	19870520
EP 246885	A3	19880622		
R: DE, FR, GB				
JP 63100440	A	19880502	JP 1987-35781	19870220
JP 2592447	B2	19970319		
JP 63100441	A	19880502	JP 1987-35782	19870220
JP 2592448	B2	19970319		
US 4925770	A	19900515	US 1988-284251	19881214
PRIORITY APPLN. INFO.:			JP 1986-113508	A 19860520
			JP 1986-138144	A 19860616
			US 1987-47187	B2 19870506

GI For diagram(s), see printed CA Issue.

AB A contrast-enhancing layer for a photolithog. material for formation of a patterned image (i.e., a resist image) by the light-projection method is comprised of a photobleachable compound having the structural unit represented by the formula I (Z = a divalent group which forms a heterocyclic aromatic ring structure with the N atom; X- = a monovalent anion; n = a pos. integer)

and a water-soluble polymer binder. Thus, a Si wafer was coated with a pos.-working photoresist composition (Microposit 1400-27), dried, overcoated with an aqueous solution containing II (a photobleachable compound) and pullulan, dried, exposed to UV (365 nm) radiation through a wafer stepper, and developed to give a line-and-space pattern (0.5  $\mu$ m width) with clear resolution

IT 113657-73-1

RL: USES (Uses)

(photobleachable contrast-enhancing layers containing, for photoresists)

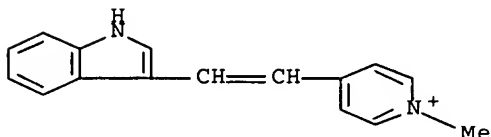
RN 113657-73-1 CAPLUS

CN Pyridinium, 4-[2-(1H-indol-3-yl)ethenyl]-1-methyl-, methyl sulfate (9CI)  
(CA INDEX NAME)

CM 1

CRN 113657-72-0

CMF C16 H15 N2



CM 2

CRN 21228-90-0

CMF C H3 O4 S

Me-O-SO<sub>3</sub><sup>-</sup>

L5 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1981:103639 CAPLUS Full-text

DOCUMENT NUMBER: 94:103639

TITLE: Isolation and synthesis of 5-ethyl-2-methyl-11H-pyrido[3,4-a]carbazolium hydroxide, a new indole alkaloid type from *Aspidosperma gilbertii*

AUTHOR(S): Miranda, Edson Conde; Brieskorn, Carl Heinz; Blechert, Siegfried

CORPORATE SOURCE: Inst. Pharm. Lebensmittelchem., Univ. Wuerzburg, Wuerzburg, D-8700, Fed. Rep. Ger.

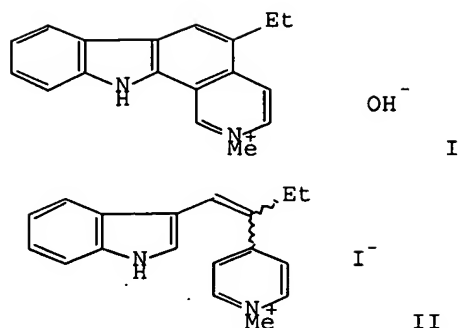
SOURCE: Chemische Berichte (1980), 113(10), 3245-8  
CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: German

GI



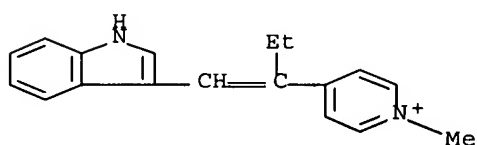


AB The indole alkaloid I was isolated from the bark of *Aspidosperma gilbertii*. I was synthesized by reaction of 3-indolecarboxaldehyde with 1-methyl-4-propylpyridinium iodide to give II, which underwent photochem cyclization.

IT 76787-85-4P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and photochem. cyclization of pyridocarbazol derivs. from)

RN 76787-85-4 CAPLUS

CN Pyridinium, 4-[1-(1H-indol-3-ylmethylene)propyl]-1-methyl-, iodide (9CI)  
 (CA INDEX NAME)



●  $\text{I}^-$

L5 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1981:64937 CAPLUS Full-text

DOCUMENT NUMBER: 94:64937

TITLE: Vinylogous anhydro bases of pyridylindoles

AUTHOR(S): Stupnikova, T. V.; Kalafat, V. N.; Klyuev, N. A.;  
 Marshtupa, V. P.; Sagitullin, R. S.

CORPORATE SOURCE: Donetsk. Gos. Univ., Donetsk, USSR

SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1980), (10),  
 1360-4  
 CODEN: KGSSAQ; ISSN: 0453-8234

DOCUMENT TYPE: Journal

LANGUAGE: Russian

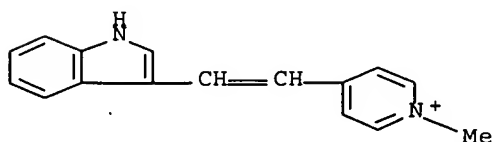
GI

AB Treatment of I (R = Me, hexyl, dodecyl), II, and III with OH- gave IV (same R), V, and VI, resp., with little or no dealkylation. The pKa values of IV-VI were 10.00-11.17; protonation by HI occurred on the indolenine N atom to give the starting iodides. Alkylation and benzylation of IV-VI also occurred on the indolenine N atom. IR, electronic, and mass spectral data were given for the anhydro bases.

IT 26608-75-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with hydroxide)

RN 26608-75-3 CAPLUS

CN Pyridinium, 4-[2-(1H-indol-3-yl)ethenyl]-1-methyl-, iodide (9CI) (CA INDEX NAME)



● I<sup>-</sup>

L5 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1977:603333 CAPLUS Full-text

DOCUMENT NUMBER: 87:203333

TITLE: Dyeing paper material

INVENTOR(S): Moeckli, Peter

PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.

SOURCE: Ger. Offen., 23 pp.  
 CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2711521	A1	19770929	DE 1977-2711521	19770316
DE 2711521	C3	19790201		
CH 601558	A5	19780714	CH 1976-3405	19760318
US 4089647	A	19780516	US 1977-767591	19770210
FI 7700795	A	19770919	FI 1977-795	19770314
FI 58532	B	19801031		
FI 58532	C	19810210		
FR 2344673	A1	19771014	FR 1977-7910	19770316
FR 2344673	B1	19800425		
CA 1107462	A1	19810825	CA 1977-274079	19770316
BE 852553	A1	19770919	BE 1977-175853	19770317
SE 7703056	A	19770919	SE 1977-3056	19770317
SE 421077	B	19811123		
SE 421077	C	19820304		
BR 7701652	A	19780103	BR 1977-1652	19770317
ES 456952	A1	19780116	ES 1977-456952	19770317
ZA 7701618	A	19780222	ZA 1977-1618	19770317

AU 7723350	A	19780921	AU 1977-23350	19770317
GB 1571927	A	19800723	GB 1977-11463	19770317
JP 54005002	B	19790313	JP 1977-29359	19770318

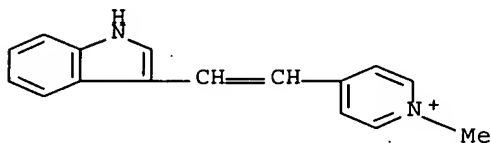
PRIORITY APPLN. INFO.: CH 1976-3405 A 19760318

AB Addition of aqueous solns. of (indolylvinyl)-N-methylpyridinium chlorides to waste paper pulps gave colored papers. Thus, 50 g waste paper in 1 L H<sub>2</sub>O was beaten to obtain a fiber suspension, diluted with 1 L H<sub>2</sub>O, treated with 1 g 20% aqueous 1-methyl-2-[(2-methyl-1-H-indol-3-yl)vinyl]pyridinium chloride [64651-41-8] solution, diluted with H<sub>2</sub>O to 0.5% consistency, formed into paper web, and dried for 5 min at 100° to give waterproof, bright yellow wrapping paper.

IT 64651-39-4P  
RL: PREP (Preparation)  
(dye for paper, manufacture of)

RN 64651-39-4 CAPLUS

CN Pyridinium, 4-[2-(1H-indol-3-yl)ethenyl]-1-methyl-, chloride (9CI) (CA INDEX NAME)



● Cl<sup>-</sup>

L5 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN ?

ACCESSION NUMBER: 1972:69480 CAPLUS Full-text

DOCUMENT NUMBER: 76:69480

TITLE: Inhibitors of choline acetyltransferase

AUTHOR(S): Cavallito, C. J.; White, Helen Lyong; Yun, H. S.

CORPORATE SOURCE: Sch. Pharm., Univ. North Carolina, Chapel Hill, NC, USA

SOURCE: Drugs Cholinergic Mech. CNS (Cent. Nerv. Syst.), Proc. Conf. (1970), 97-116. Editor(s): Heilbronn, Edith. Foersvarets Forskningsanst.: Stockholm, Swed. CODEN: 24HKAN

DOCUMENT TYPE: Conference

LANGUAGE: English

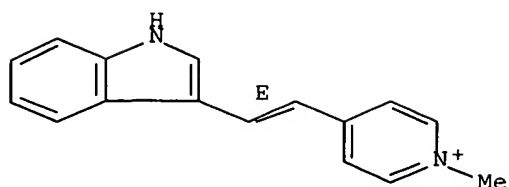
AB Choline acetyltransferase (ChAc) inhibitors were investigated. Results indicated that styrylpyridine derivs. and analogs are effective inhibitors. The structural and electronic features of the inhibitors are discussed. The inhibitors appear to block the transfer of acetyl from the acetyl CoA-ChAc complex to choline.

IT 36098-33-6  
RL: BIOL (Biological study)  
(choline acetyltransferase inhibition by)

RN 36098-33-6 CAPLUS

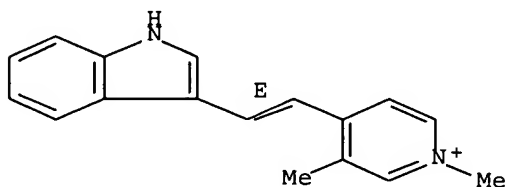
CN Pyridinium, 4-[(1E)-2-(1H-indol-3-yl)ethenyl]-1-methyl-, iodide (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L5 ANSWER 9 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1970:505755 CAPLUS Full-text  
 DOCUMENT NUMBER: 73:105755  
 TITLE: Choline acetyltransferase inhibitors. Physicochemical properties in relation to inhibitory activity of styrylpyridine analogs  
 AUTHOR(S): Allen, Richard Charles; Carlson, Gerald L.; Cavallito, C. J.  
 CORPORATE SOURCE: Sch. of Pharm., Univ. of North Carolina, Chapel Hill, NC, USA  
 SOURCE: Journal of Medicinal Chemistry (1970), 13(5), 909-12  
 CODEN: JMCMAR; ISSN: 0022-2623  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Hueckel MO and Hansch calcns. were performed on various styrylpyridine derivs., some of which are potent inhibitors of choline acetyltransferase. These compds. apparently bind the enzyme by hydrophobic and  $\pi$  donor contributions of the aryl moiety, and  $\pi$  acceptor interactions, presumably by the pyridinium-like portion.  
 IT 29714-15-6  
 RL: PRP (Properties)  
 (mol. orbitals of, choline acetyltransferase inhibition in relation to)  
 RN 29714-15-6 CAPLUS  
 CN Pyridinium, 4-[(1E)-2-(1H-indol-3-yl)ethenyl]-1,3-dimethyl-, iodide (9CI)  
 (CA INDEX NAME)

Double bond geometry as shown.



L5 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1970:107348 CAPLUS Full-text

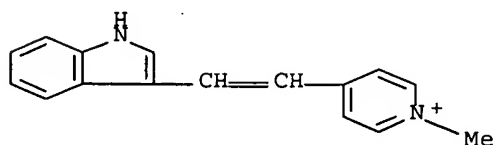
DOCUMENT NUMBER: 72:107348  
TITLE: Choline acetyltransferase inhibitors. Dimensional and  
substituent effects among styrylpyridine analogs  
AUTHOR(S): Cavallito, Chester J.; Yun, H. S.; Kaplan, T.; Smith,  
John Crispin; Foldes, Francis F.  
CORPORATE SOURCE: Sch. of Pharm., Univ. of North Carolina, Chapel Hill,  
NC, USA  
SOURCE: Journal of Medicinal Chemistry (1970), 13(2), 221-4  
CODEN: JMCMAR; ISSN: 0022-2623  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Among styrylpyridine analogs, choline acetylase (ChA) inhibitory potency is diminished by highly electroneg. substituents (CN, NO<sub>2</sub>) on the 3- or 4-position of the phenyl ring but is enhanced by halogens (Cl, Br) less electroneg. than F. Substituents inducing deviation from coplanarity of the 2 ring systems are unfavorable for inhibitory activity. 3-Methyl substitution on the pyridine ring enhances potency. The nature of the pyrido-N-attached quaternizing group is noncritical and a hydrophilic substituent can provide potent, more water-soluble, derivs. A naphthyl vinyl-quinoline system provides a high order of potency, but the same mass distributed as in phenanthrylvinylpyridine is unfavorable. ChA inhibitory activity among these compds. seems favored by thin flat mols., one end of which tends to have  $\pi$ -electron-excessive, the other end  $\pi$ -electron-deficient, characteristics separated by a conjugating exocyclic bond. The photolability of some of these compds. in solution requires appropriate precautionary measures in their evaluation.

IT 26608-75-3  
RL: BIOL (Biological study)  
(choline acetyltransferase inhibition by)

RN 26608-75-3 CAPLUS

CN Pyridinium, 4-[2-(1H-indol-3-yl)ethenyl]-1-methyl-, iodide (9CI) (CA INDEX NAME)



● I<sup>-</sup>

L5 ANSWER 11 OF 16 USPATFULL on STN

ACCESSION NUMBER: 2001:66940 USPATFULL Full-text

TITLE: Oxidation dyeing composition for keratin fibres and  
dyeing method using said composition

INVENTOR(S): de la Mettrie, Roland, Le Vesinet, France  
Cotteret, Jean, Verneuil-sur-Seine, France  
de Labbey, Arnaud, Aulnay Sous Bois, France  
Maubru, Mireille, Chatou, France

PATENT ASSIGNEE(S): L'Oreal S.A., Paris, France (non-U.S. corporation)

NUMBER	KIND	DATE
-----		

PATENT INFORMATION: US 6228129 B1 20010508  
 WO 9917730 19990415  
 APPLICATION INFO.: US 1999-319166 19990701 (9)  
 WO 1998-FR2075 19980928  
 19990701 PCT 371 date  
 19990701 PCT 102(e) date

	NUMBER	DATE
PRIORITY INFORMATION:	FR 1997-12353	19971003
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	Granted	
PRIMARY EXAMINER:	Liott, Caroline D.	
LEGAL REPRESENTATIVE:	Finnegan, Henderson, Farabow, Garrett & Dunner, L.L.P.	
NUMBER OF CLAIMS:	52	
EXEMPLARY CLAIM:	1	
LINE COUNT:	1560	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The invention relates to a ready-to-use composition for the oxidation dyeing of keratin fibers, and in particular human keratin fibers such as the hair, comprising, in a medium which is suitable for dyeing, at least one oxidation base, at least one cationic direct dye and at least one enzyme of 2-electron oxidoreductase type in the presence of at least one donor for the said enzyme, and to the dyeing process using this composition.

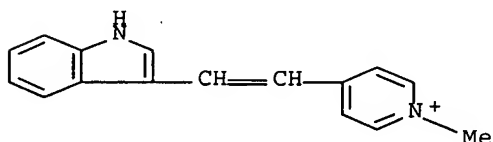
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 64651-39-4

(oxidative hair dye compns. containing oxidoreductase-type enzymes, oxidation bases, and direct cationic dyes)

RN 64651-39-4 USPATFULL

CN Pyridinium, 4-[2-(1H-indol-3-yl)ethenyl]-1-methyl-, chloride (9CI) (CA INDEX NAME)



● C1 -

L5 ANSWER 12 OF 16 USPATFULL on STN

ACCESSION NUMBER: 1999:162994 USPATFULL Full-text

TITLE: Compositions and processes for dyeing keratin fibers with cationic direct dyes, oxidation bases, and oxidizing agents

INVENTOR(S): Rondeau, Christine, Sartrouville, France  
 Cotteret, Jean, Verneuil Sur Seine, France  
 De La Mettrie, Roland, Le Vesinet, France

PATENT ASSIGNEE(S): L'Oreal, Paris, France (non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 6001135		19991214
APPLICATION INFO.:	US 1997-994444		19971219 (8)

	NUMBER	DATE
PRIORITY INFORMATION:	FR 1996-15895	19961223
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	Granted	
PRIMARY EXAMINER:	Liott, Caroline D.	
LEGAL REPRESENTATIVE:	Finnegan, Henderson, Farabow, Garrett & Dunner, L.L.P.	
NUMBER OF CLAIMS:	41	
EXEMPLARY CLAIM:	1	
LINE COUNT:	823	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB A ready-to-use composition for the oxidation dyeing of keratin fibers, in particular human keratin fibers such as the hair, this ready-to-use composition comprising at least one oxidation base in combination with at least one selected cationic direct dye and at least one oxidizing agent, as well as to the dyeing process using this ready-to-use composition.

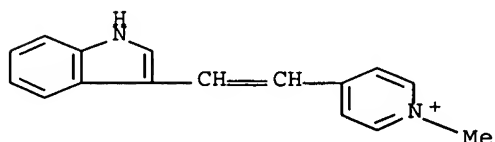
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 64651-39-4

(cationic direct colorant; oxidative hair dye compns. containing cationic direct colorants with good coloration, shine, and shampoo resistance)

RN 64651-39-4 USPATFULL

CN Pyridinium, 4-[2-(1H-indol-3-yl)ethenyl]-1-methyl-, chloride (9CI) (CA INDEX NAME)



● Cl<sup>-</sup>

L5 ANSWER 13 OF 16 USPATFULL on STN

ACCESSION NUMBER: 1999:154874 USPATFULL Full-text

TITLE: Composition for the oxidation dyeing of keratin fibers containing a cationic direct dye and dyeing process using this composition

INVENTOR(S): Rondeau, Christine, Sartrouville, France  
Cotteret, Jean, Verneuil Sur Seine, France  
de la Mettrie, Roland, le Vesinet, France

PATENT ASSIGNEE(S): L'Oreal, France (non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 5993490		19991130
APPLICATION INFO.:	US 1997-994130		19971219 (8)

	NUMBER	DATE
PRIORITY INFORMATION:	FR 1996-15891	19961223
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	Granted	
PRIMARY EXAMINER:	Liott, Caroline D.	
LEGAL REPRESENTATIVE:	Finnegan, Henderson, Farabow, Garrett & Dunner, L.L.P.	
NUMBER OF CLAIMS:	41	
EXEMPLARY CLAIM:	1	
LINE COUNT:	768	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB A ready-to-use composition for the oxidation dyeing of keratin fibers, in particular human keratin fibers such as the hair, comprising at least one oxidation base selected from para-phenylenediamines and bis(phenyl)alkylenediamines, in combination with at least one coupler selected from meta-diphenols, at least one selected cationic direct dye and at least one oxidizing agent, as well as to the dyeing process using this composition.

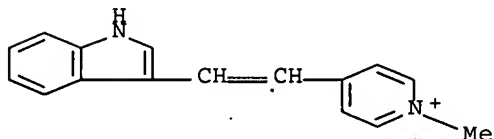
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 64651-39-4

(cationic direct dye; oxidative hair dye compns. with good coloration and shampoo resistance)

RN 64651-39-4 USPATFULL

CN Pyridinium, 4-[2-(1H-indol-3-yl)ethenyl]-1-methyl-, chloride (9CI) (CA INDEX NAME)



● Cl<sup>-</sup>

L5 ANSWER 14 OF 16 USPATFULL on STN

ACCESSION NUMBER: 1998:33383 USPATFULL Full-text

TITLE: Process for dyeing keratin-containing fibres with cationic dyes

INVENTOR(S): Mockli, Peter, Sandgrubenstrasse, Switzerland

PATENT ASSIGNEE(S): Ciba Specialty Chemicals Corporation, Tarrytown, NY, United States (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 5733343		19980331
APPLICATION INFO.:	US 1996-756448		19961126 (8)
RELATED APPLN. INFO.:	Continuation of Ser. No. US 1995-392783, filed on 28 Feb 1995, now abandoned		

NUMBER	DATE
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PRIORITY INFORMATION: CH 1993-2020 19930705  
DOCUMENT TYPE: Utility  
FILE SEGMENT: Granted  
PRIMARY EXAMINER: Lieberman, Paul  
ASSISTANT EXAMINER: Dusheck, Caroline L.  
LEGAL REPRESENTATIVE: Mansfield, Kevin T.  
NUMBER OF CLAIMS: 22  
EXEMPLARY CLAIM: 1  
LINE COUNT: 691

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Keratin-containing fibres, in particular human hair, are dyed using dyes of formulae (1) to (6) indicated in claim 1. These dyes make it possible to dye by the trichromatic principle even in dark shades.

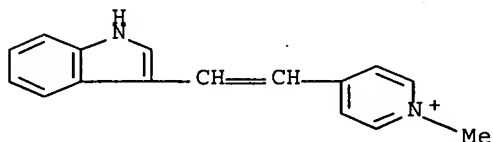
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 64651-39-4

(hair dyeing prepns. containing cationic dyes)

RN 64651-39-4 USPATFULL

CN Pyridinium, 4-[2-(1H-indol-3-yl)ethenyl]-1-methyl-, chloride (9CI) (CA INDEX NAME)



● Cl<sup>-</sup>

L5 ANSWER 15 OF 16 USPATFULL on STN

ACCESSION NUMBER: 90:38343 USPATFULL Full-text

TITLE: Contrast-enhancing agent for photolithography

INVENTOR(S): Ichimura, Kunihiro, Tsukuba, Japan  
Yonezawa, Teruhiko, Kanagawa, Japan  
Kikuchi, Hideo, Chiba, Japan  
Tochizawa, Nariaki, Funabashi, Japan  
Hayashi, Keiichi, Funabashi, Japan

PATENT ASSIGNEE(S): Director General of Agency of Industrial Science and Technology, Tokyo, Japan (non-U.S. government)  
Toyo Gosei Kogyo Co., Ltd., Chiba, Japan (non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 4925770		19900515
APPLICATION INFO.:	US 1988-284251		19881214 (7)
RELATED APPLN. INFO.:	Continuation-in-part of Ser. No. US 1987-47187, filed on 6 May 1987, now abandoned		

NUMBER	DATE
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PRIORITY INFORMATION: JP 1986-113508 19860520  
 JP 1986-138144 19860616  
 DOCUMENT TYPE: Utility  
 FILE SEGMENT: Granted  
 PRIMARY EXAMINER: Michl, Paul R.  
 ASSISTANT EXAMINER: Buscher, Mark R.  
 LEGAL REPRESENTATIVE: Hopgood, Calimafde, Kalil, Blaustein & Judlowe  
 NUMBER OF CLAIMS: 7  
 EXEMPLARY CLAIM: 1  
 LINE COUNT: 972  
 CAS INDEXING IS AVAILABLE FOR THIS PATENT.

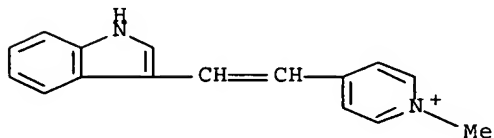
AB The invention provides a novel contrast-enhancing agent for photolithography which is used as an overcoating on a positive-working photoresist layer for enhancing the contrast of the photoresist in a low-contrast exposure to light. The composition comprises, in addition to a watersoluble polymer, e.g., poly(vinyl alcohol), poly(vinyl pyrrolidone) and pullulan, as the binder, a specific photo-bleachable organic compound having, in a molecule, at least one nitrogen-containing heterocyclic aromatic structure represented by the general formula ##STR1## in which Z is a divalent group to form the heterocyclic aromatic ring with the nitrogen atom, X is an anionic group of monovalency and n is a positive integer of, e.g., 1 or 2.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 113657-73-1  
 (photobleachable contrast-enhancing layers containing, for photoresists)  
 RN 113657-73-1 USPATFULL  
 CN Pyridinium, 4-[2-(1H-indol-3-yl)ethenyl]-1-methyl-, methyl sulfate (9CI)  
 (CA INDEX NAME)

CM 1

CRN 113657-72-0  
 CMF C16 H15 N2



CM 2

CRN 21228-90-0  
 CMF C H3 O4 S

Me-O-SO<sub>3</sub><sup>-</sup>

ACCESSION NUMBER: 78:25171 USPATFULL Full-text  
 TITLE: Process for the dyeing of paper material  
 INVENTOR(S): Mockli, Peter, Basel, Switzerland  
 PATENT ASSIGNEE(S): Ciba-Geigy AG, Basel, Switzerland (non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 4089647		19780516
APPLICATION INFO.:	US 1977-767591		19770210 (5)

	NUMBER	DATE
PRIORITY INFORMATION:	CH 1976-3405	19760318
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	Granted	
PRIMARY EXAMINER:	Schofer, Joseph L.	
ASSISTANT EXAMINER:	Tungol, Maria S.	
LEGAL REPRESENTATIVE:	Roberts, Edward McC., Almaula, Probodh I.	
NUMBER OF CLAIMS:	13	
EXEMPLARY CLAIM:	1	
LINE COUNT:	287	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB A process for the dyeing of paper material from an aqueous medium, comprising the use of at least one water-soluble dye of the formula ##STR1## wherein Py represents a pyridyl group of the formula ##STR2## R.sub.1 represents lower alkyl, substituted lower alkyl, allyl, or benzyl, R.sub.2 represents hydrogen, halogen, methyl or ethyl,

R.sub.3 represents hydrogen, methyl, ethyl or phenyl,

R.sub.4 represents hydrogen, lower alkyl substituted lower alkyl, or allyl, and

A.crc1bar. represents an anion.

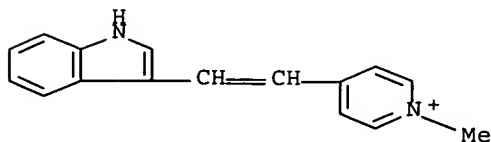
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 64651-39-4P

(dye for paper, manufacture of)

RN 64651-39-4 USPATFULL

CN Pyridinium, 4-[2-(1H-indol-3-yl)ethenyl]-1-methyl-, chloride (9CI) (CA INDEX NAME)



● Cl<sup>-</sup>

=> s l4 and "cell proliferation"  
L6 1 L4 AND "CELL PROLIFERATION"

=> d l6 ibib, abs, hitstr  
'HITSTR' IS NOT A VALID FORMAT FOR FILE 'MEDLINE'

ENTER DISPLAY FORMAT (BIB):ibib, abs

L6 ANSWER 1 OF 1 MEDLINE on STN  
ACCESSION NUMBER: 2006351356 MEDLINE Full-text  
DOCUMENT NUMBER: PubMed ID: 16766262  
TITLE: Attenuation of LDH-A expression uncovers a link between glycolysis, mitochondrial physiology, and tumor maintenance.  
AUTHOR: Fantin Valeria R; St-Pierre Julie; Leder Philip  
CORPORATE SOURCE: Department of Genetics, Harvard Medical School and Howard Hughes Medical Institute, Boston, Massachusetts 02115, USA.  
SOURCE: Cancer cell, (2006 Jun) Vol. 9, No. 6, pp. 425-34.  
Journal code: 101130617. ISSN: 1535-6108.  
PUB. COUNTRY: United States  
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)  
LANGUAGE: English  
FILE SEGMENT: Priority Journals  
ENTRY MONTH: 200608  
ENTRY DATE: Entered STN: 13 Jun 2006  
Last Updated on STN: 10 Aug 2006  
Entered Medline: 9 Aug 2006

AB Alterations in cellular metabolism are among the most consistent hallmarks of cancer. Herein we have investigated the relationship between increased aerobic lactate production and mitochondrial physiology in tumor cells. To diminish the ability of malignant cells to metabolize pyruvate to lactate, lactate dehydrogenase A (LDH-A) levels were knocked down by means of LDH-A short hairpin RNAs. Reduction in LDH-A activity resulted in stimulation of mitochondrial respiration and decrease of mitochondrial membrane potential. It also compromised the ability of these tumor cells to proliferate under hypoxia. The tumorigenicity of the LDH-A-deficient cells was severely diminished, and this phenotype was reversed by complementation with the human ortholog LDH-A protein. These results demonstrate that LDH-A plays a key role in tumor maintenance.

=> d his

(FILE 'HOME' ENTERED AT 15:58:45 ON 26 JAN 2007)

FILE 'REGISTRY' ENTERED AT 15:59:02 ON 26 JAN 2007

L1 STRUCTURE UPLOADED  
L2 2 S L1  
L3 27 S L1 FULL

FILE 'MEDLINE, CAPLUS, WPIDS, USPATFULL' ENTERED AT 15:59:33 ON 26 JAN 2007

L4 58 S L3  
L5 16 S L4 NOT PY>2001  
L6 1 S L4 AND "CELL PROLIFERATION"

=> s 14 and "cancer"

L7 3 L4 AND "CANCER"

=> d 17 1-3 ibib, abs, hitstr

ENTER DISPLAY FORMAT (BIB):abs, ibib

L7 ANSWER 1 OF 3 MEDLINE on STN

AB Alterations in cellular metabolism are among the most consistent hallmarks of cancer. Herein we have investigated the relationship between increased aerobic lactate production and mitochondrial physiology in tumor cells. To diminish the ability of malignant cells to metabolize pyruvate to lactate, lactate dehydrogenase A (LDH-A) levels were knocked down by means of LDH-A short hairpin RNAs. Reduction in LDH-A activity resulted in stimulation of mitochondrial respiration and decrease of mitochondrial membrane potential. It also compromised the ability of these tumor cells to proliferate under hypoxia. The tumorigenicity of the LDH-A-deficient cells was severely diminished, and this phenotype was reversed by complementation with the human ortholog LDH-A protein. These results demonstrate that LDH-A plays a key role in tumor maintenance.

ACCESSION NUMBER: 2006351356 MEDLINE Full-text

DOCUMENT NUMBER: PubMed ID: 16766262

TITLE: Attenuation of LDH-A expression uncovers a link between glycolysis, mitochondrial physiology, and tumor maintenance.

AUTHOR: Fantin Valeria R; St-Pierre Julie; Leder Philip

CORPORATE SOURCE: Department of Genetics, Harvard Medical School and Howard Hughes Medical Institute, Boston, Massachusetts 02115, USA.

SOURCE: Cancer cell, (2006 Jun) Vol. 9, No. 6, pp. 425-34.  
Journal code: 101130617. ISSN: 1535-6108.

PUB. COUNTRY: United States

DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)

LANGUAGE: English

FILE SEGMENT: Priority Journals

ENTRY MONTH: 200608

ENTRY DATE: Entered STN: 13 Jun 2006

Last Updated on STN: 10 Aug 2006

Entered Medline: 9 Aug 2006

L7 ANSWER 2 OF 3 MEDLINE on STN

AB Tumorigenesis results from events that impinge on a variety of collaborating metabolic pathways. To assess their role in this process, we utilized a cell-based assay to perform a high-throughput, chemical library screen. In so doing, we identified F16, a small molecule that selectively inhibits proliferation of mammary epithelial, neu-overexpressing cells, as well as a variety of mouse mammary tumor and human breast cancer cell lines. F16 belongs to a group of structurally similar molecules with a delocalized positive charge. The compound is accumulated in mitochondria of responsive cells, driven by the membrane potential, and it compromises their functional integrity. Mitochondrial hyperpolarization is a shared feature of many tumor cell lines, explaining the broad action spectrum of this novel delocalized lipophilic cation.

ACCESSION NUMBER: 2002401591 MEDLINE Full-text

DOCUMENT NUMBER: PubMed ID: 12150823

TITLE: A novel mitochondriotoxic small molecule that selectively inhibits tumor cell growth.

AUTHOR: Fantin Valeria R; Berardi Marcelo J; Scorrano Luca;  
Korsmeyer Stanley J; Leder Philip

CORPORATE SOURCE: Department of Genetics, Harvard Medical School, Boston,

Massachusetts 02115, USA.  
SOURCE: Cancer cell, (2002 Jul) Vol. 2, No. 1, pp. 29-42.  
Journal code: 101130617. ISSN: 1535-6108.  
PUB. COUNTRY: United States  
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)  
LANGUAGE: English  
FILE SEGMENT: Priority Journals  
ENTRY MONTH: 200303  
ENTRY DATE: Entered STN: 2 Aug 2002  
Last Updated on STN: 26 Mar 2003  
Entered Medline: 25 Mar 2003

L7 ANSWER 3 OF 3 MEDLINE on STN

AB Mitochondria are principal actors in apoptosis as central hubs for diverse apoptotic signals. A new paper demonstrates the therapeutic potential of directly engaging these apoptotic pathways by identifying a mitochondrial toxin selective for tumor cells.

ACCESSION NUMBER: 2002401587 MEDLINE Full-text  
DOCUMENT NUMBER: PubMed ID: 12150816  
TITLE: A mitochondrial Achilles' heel in cancer?.  
AUTHOR: Hockenbery David M  
CORPORATE SOURCE: Fred Hutchinson Cancer Research Center, Seattle, Washington 98109, USA.. dhockenb@fhcrc.org  
SOURCE: Cancer cell, (2002 Jul) Vol. 2, No. 1, pp. 1-2.  
Journal code: 101130617. ISSN: 1535-6108.  
PUB. COUNTRY: United States  
DOCUMENT TYPE: Commentary  
Journal; Article; (JOURNAL ARTICLE)  
LANGUAGE: English  
FILE SEGMENT: Priority Journals  
ENTRY MONTH: 200303  
ENTRY DATE: Entered STN: 2 Aug 2002  
Last Updated on STN: 26 Mar 2003  
Entered Medline: 25 Mar 2003

=> d his

(FILE 'HOME' ENTERED AT 15:58:45 ON 26 JAN 2007)

FILE 'REGISTRY' ENTERED AT 15:59:02 ON 26 JAN 2007

L1 STRUCTURE UPLOADED

L2 2 S L1

L3 27 S L1 FULL

FILE 'MEDLINE, CAPLUS, WPIDS, USPATFULL' ENTERED AT 15:59:33 ON 26 JAN 2007

L4 58 S L3

L5 16 S L4 NOT PY>2001

L6 1 S L4 AND "CELL PROLIFERATION"

L7 3 S L4 AND "CANCER"

=>

---Logging off of STN---

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Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	112.70	285.01
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-7.80	-7.80

STN INTERNATIONAL LOGOFF AT 16:05:25 ON 26 JAN 2007

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=> file registry

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

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0.21

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DICTIONARY FILE UPDATES: 25 JAN 2007 HIGHEST RN 918475-45-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

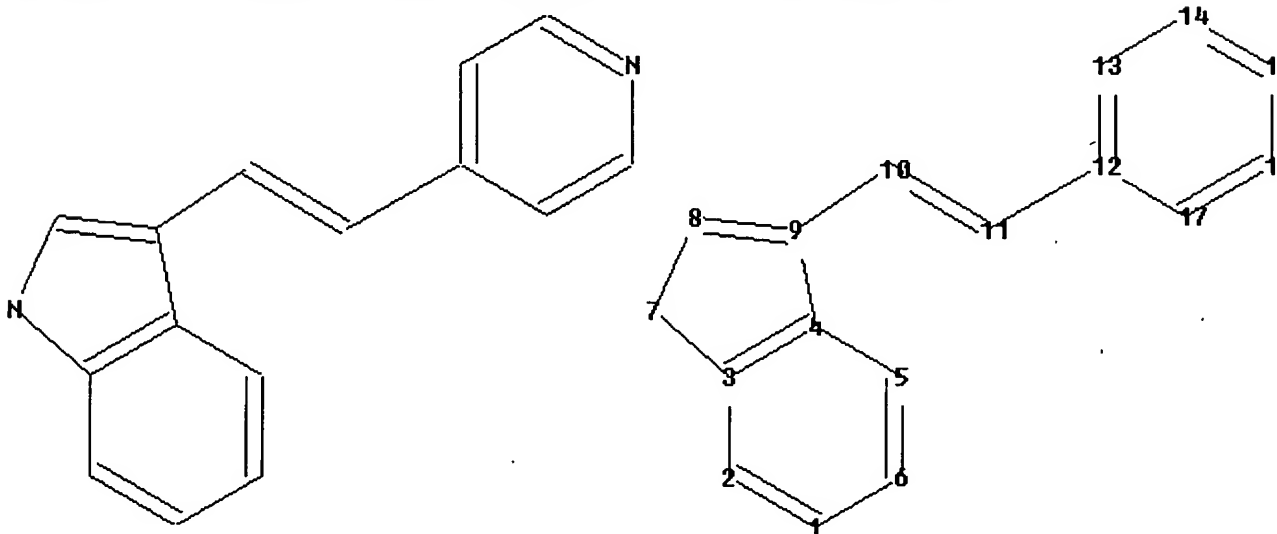
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

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Uploading C:\Program Files\Stnexp\Queries\10613762\_genus.str



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ring nodes :

1 2 3 4 5 6 7 8 9 12 13 14 15 16 17

chain bonds :

9-10 10-11 11-12

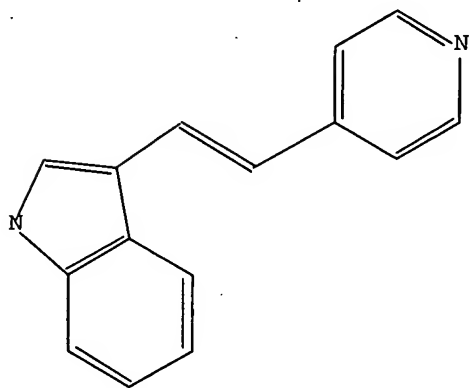


ring bonds :  
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 16-17  
 exact/norm bonds :  
 3-7 4-9 7-8 8-9  
 exact bonds :  
 9-10 10-11 11-12  
 normalized bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6 12-13 12-17 13-14 14-15 15-16 16-17

Match level :  
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS  
 11:CLASS 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom

L1 STRUCTURE UPLOADED

=> d 11  
 L1 HAS NO ANSWERS  
 L1 STR



Structure attributes must be viewed using STN Express query preparation.

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 SAMPLE SCREEN SEARCH COMPLETED - 313 TO ITERATE  
  
 100.0% PROCESSED 313 ITERATIONS 9 ANSWERS  
 SEARCH TIME: 00.00.01  
  
 FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 5199 TO 7321  
 PROJECTED ANSWERS: 9 TO 360

L2 9 SEA SSS SAM L1

=> s 11 full

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FULL SCREEN SEARCH COMPLETED - 6177 TO ITERATE

100.0% PROCESSED 6177 ITERATIONS 127 ANSWERS  
SEARCH TIME: 00.00.01

L3 127 SEA SSS FUL L1

=> file medline, caplus, wpids, uspatfull

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	172.10	172.31

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FILE 'CAPLUS' ENTERED AT 16:07:29 ON 26 JAN 2007  
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FILE 'USPATFULL' ENTERED AT 16:07:29 ON 26 JAN 2007  
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=> s 13

SAMPLE SEARCH INITIATED 16:07:35 FILE 'WPIDS'  
SAMPLE SCREEN SEARCH COMPLETED - 11 TO ITERATE

100.0% PROCESSED 11 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 11 TO 209  
PROJECTED ANSWERS: 0 TO 0

L4 95 L3

=> s 14 and "cell proliferation"

L5 1 L4 AND "CELL PROLIFERATION"

=> d 15 ibib, abs

L5 ANSWER 1 OF 1 MEDLINE on STN  
ACCESSION NUMBER: 2006351356 MEDLINE Full-text  
DOCUMENT NUMBER: PubMed ID: 16766262  
TITLE: Attenuation of LDH-A expression uncovers a link between glycolysis, mitochondrial physiology, and tumor maintenance.  
AUTHOR: Fantin Valeria R; St-Pierre Julie; Leder Philip  
CORPORATE SOURCE: Department of Genetics, Harvard Medical School and Howard Hughes Medical Institute, Boston, Massachusetts 02115, USA.  
SOURCE: Cancer cell, (2006 Jun) Vol. 9, No. 6, pp. 425-34.  
Journal code: 101130617. ISSN: 1535-6108.  
PUB. COUNTRY: United States  
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)  
LANGUAGE: English  
FILE SEGMENT: Priority Journals

ENTRY MONTH: 200608  
ENTRY DATE: Entered STN: 13 Jun 2006  
Last Updated on STN: 10 Aug 2006  
Entered Medline: 9 Aug 2006

AB Alterations in cellular metabolism are among the most consistent hallmarks of cancer. Herein we have investigated the relationship between increased aerobic lactate production and mitochondrial physiology in tumor cells. To diminish the ability of malignant cells to metabolize pyruvate to lactate, lactate dehydrogenase A (LDH-A) levels were knocked down by means of LDH-A short hairpin RNAs. Reduction in LDH-A activity resulted in stimulation of mitochondrial respiration and decrease of mitochondrial membrane potential. It also compromised the ability of these tumor cells to proliferate under hypoxia. The tumorigenicity of the LDH-A-deficient cells was severely diminished, and this phenotype was reversed by complementation with the human ortholog LDH-A protein. These results demonstrate that LDH-A plays a key role in tumor maintenance.

=> d his

(FILE 'HOME' ENTERED AT 16:06:43 ON 26 JAN 2007)

FILE 'REGISTRY' ENTERED AT 16:06:55 ON 26 JAN 2007

L1 STRUCTURE UPLOADED  
L2 9 S L1  
L3 127 S L1 FULL

FILE 'MEDLINE, CAPLUS, WPIDS, USPATFULL' ENTERED AT 16:07:29 ON 26 JAN 2007

L4 95 S L3  
L5 1 S L4 AND "CELL PROLIFERATION"

=> s l4 and "differentiation"

L6 0 L4 AND "DIFFERENTIATION"

=> s l4 and "tumor"

L7 5 L4 AND "TUMOR"

=> d l7 1-5 ibib, abs, hitstr

L7 ANSWER 1 OF 5 MEDLINE on STN

ACCESSION NUMBER: 2006351356 MEDLINE Full-text

DOCUMENT NUMBER: PubMed ID: 16766262

TITLE: Attenuation of LDH-A expression uncovers a link between glycolysis, mitochondrial physiology, and tumor maintenance.

AUTHOR: Fantin Valeria R; St-Pierre Julie; Leder Philip

CORPORATE SOURCE: Department of Genetics, Harvard Medical School and Howard Hughes Medical Institute, Boston, Massachusetts 02115, USA.

SOURCE: Cancer cell, (2006 Jun) Vol. 9, No. 6, pp. 425-34.

Journal code: 101130617. ISSN: 1535-6108.

PUB. COUNTRY: United States

DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)

LANGUAGE: English

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L7 ANSWER 2 OF 5 MEDLINE on STN  
ACCESSION NUMBER: 2004029169 MEDLINE Full-text  
DOCUMENT NUMBER: PubMed ID: 14729642  
TITLE: F16, a mitochondriotoxic compound, triggers apoptosis or

necrosis depending on the genetic background of the target carcinoma cell.

AUTHOR: Fantin Valeria R; Leder Philip  
CORPORATE SOURCE: Department of Genetics, Harvard Medical School and Howard Hughes Medical Institute, Boston, Massachusetts 02115, USA.  
SOURCE: Cancer research, (2004 Jan 1) Vol. 64, No. 1, pp. 329-36.  
Journal code: 2984705R. ISSN: 0008-5472.

PUB. COUNTRY: United States  
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)  
LANGUAGE: English  
FILE SEGMENT: Priority Journals  
ENTRY MONTH: 200404  
ENTRY DATE: Entered STN: 21 Jan 2004  
Last Updated on STN: 2 Apr 2004  
Entered Medline: 1 Apr 2004

AB Mutations that lead to the emergence of resistance to apoptosis are commonly observed among tumor cells. Some of the proteins affected are integral parts of the apoptotic cascade such as pro- and antiapoptotic members of the Bcl-2 family. F16 is a small molecule that accumulates in mitochondria of a variety of tumor cells and interferes with their physiological function. Because this interference ultimately triggers apoptosis in many affected cell lines, we examined the effect of antiapoptotic Bcl-2 overexpression on the response of cells to F16. Our results showed that high levels of Bcl-2 did not block the ability of F16 to induce cell death. However, unlike the apoptotic response that followed F16 treatment of cells with moderate Bcl-2 levels, cells resistant to a variety of apoptotic stimuli by virtue of Bcl-2 overexpression succumbed to F16 by necrosis. Thus, this dual ability of the mitochondriotoxic compound F16 to induce apoptosis and necrosis may represent an added advantage by expanding its spectrum of action toward genetically altered tumor cells incapable of apoptosis.

L7 ANSWER 3 OF 5 MEDLINE on STN  
ACCESSION NUMBER: 2002401591 MEDLINE Full-text  
DOCUMENT NUMBER: PubMed ID: 12150823  
TITLE: A novel mitochondriotoxic small molecule that selectively

inhibits tumor cell growth.

AUTHOR: Fantin Valeria R; Berardi Marcelo J; Scorrano Luca;  
Korsmeyer Stanley J; Leder Philip  
CORPORATE SOURCE: Department of Genetics, Harvard Medical School, Boston, Massachusetts 02115, USA.

SOURCE: Cancer cell, (2002 Jul) Vol. 2, No. 1, pp. 29-42.  
Journal code: 101130617. ISSN: 1535-6108.  
PUB. COUNTRY: United States  
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)  
LANGUAGE: English  
FILE SEGMENT: Priority Journals  
ENTRY MONTH: 200303  
ENTRY DATE: Entered STN: 2 Aug 2002  
Last Updated on STN: 26 Mar 2003  
Entered Medline: 25 Mar 2003

AB Tumorigenesis results from events that impinge on a variety of collaborating metabolic pathways. To assess their role in this process, we utilized a cell-based assay to perform a high-throughput, chemical library screen. In so doing, we identified F16, a small molecule that selectively inhibits proliferation of mammary epithelial, neu-overexpressing cells, as well as a variety of mouse mammary tumor and human breast cancer cell lines. F16 belongs to a group of structurally similar molecules with a delocalized positive charge. The compound is accumulated in mitochondria of responsive cells, driven by the membrane potential, and it compromises their functional integrity. Mitochondrial hyperpolarization is a shared feature of many tumor cell lines, explaining the broad action spectrum of this novel delocalized lipophilic cation.

L7 ANSWER 4 OF 5 MEDLINE on STN  
ACCESSION NUMBER: 2002401587 MEDLINE Full-text  
DOCUMENT NUMBER: PubMed ID: 12150816  
TITLE: A mitochondrial Achilles' heel in cancer?.  
AUTHOR: Hockenbery David M  
CORPORATE SOURCE: Fred Hutchinson Cancer Research Center, Seattle, Washington  
98109, USA.. dhockenb@fhcrc.org  
SOURCE: Cancer cell, (2002 Jul) Vol. 2, No. 1, pp. 1-2.  
Journal code: 101130617. ISSN: 1535-6108.  
PUB. COUNTRY: United States  
DOCUMENT TYPE: Commentary  
Journal; Article; (JOURNAL ARTICLE)  
LANGUAGE: English  
FILE SEGMENT: Priority Journals  
ENTRY MONTH: 200303  
ENTRY DATE: Entered STN: 2 Aug 2002  
Last Updated on STN: 26 Mar 2003  
Entered Medline: 25 Mar 2003

AB Mitochondria are principal actors in apoptosis as central hubs for diverse apoptotic signals. A new paper demonstrates the therapeutic potential of directly engaging these apoptotic pathways by identifying a mitochondrial toxin selective for tumor cells.

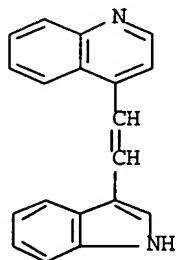
L7 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1965:416812 CAPLUS Full-text  
DOCUMENT NUMBER: 63:16812  
ORIGINAL REFERENCE NO.: 63:2952a-b  
TITLE: Styrylquinoline analogs from heterocyclic  
carboxaldehydes  
AUTHOR(S): Bahner, Carl Tabb; Kinder, Harold; Gutman, Lee  
CORPORATE SOURCE: Carson-Newman Coll., Jefferson City, TN  
SOURCE: Journal of Medicinal Chemistry (1965), 8(3), 397-8  
CODEN: JMCMAR; ISSN: 0022-2623  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Indole-3-carboxaldehyde, pyridine-3-carboxaldehyde, thiophene-2-carboxaldehyde, and N-methyl-1,2,3,4-tetrahydroquinoline-6-carboxaldehyde were used to prepare a series of quinoline and isoquinoline derivs. which were studied for antitumor activity in relation to structure. 3-(3H-Indol-3-ylidenemethyl)indole, 2-methyl-3-[(2-methyl-3H-indol-3-ylidene)-methyl]indole, and 2-methyl-3-[1-(2-methyl-3H-indol-3-ylidene)-ethyl]indole showed greater antitumor activity against KB tumor cells than 2,2',2''-methylidynetris[3-methylindole], 3,3',3''-methylidynettriindole, or 3,3',3''-methylidynetris[2-methylindole]. The greater antitumor activity in the former group is believed to be due to the double bond joining the 2 ring systems.

IT 1586-46-5P, Quinoline, 4-(2-indol-3-ylvinyl)- 1586-49-8P  
 , Quinoline, 4-[2-(1-methylindol-3-yl)vinyl]-  
 RL: PREP (Preparation)  
 (preparation of)

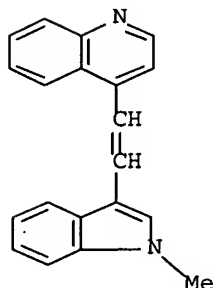
RN 1586-46-5 CAPLUS

CN Quinoline, 4-(2-indol-3-ylvinyl)- (7CI, 8CI) (CA INDEX NAME)



RN 1586-49-8 CAPLUS

CN Quinoline, 4-[2-(1-methylindol-3-yl)vinyl]- (7CI, 8CI) (CA INDEX NAME)



=> d his

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FILE 'REGISTRY' ENTERED AT 16:06:55 ON 26 JAN 2007

L1 STRUCTURE UPLOADED  
 L2 9 S L1  
 L3 127 S L1 FULL

FILE 'MEDLINE, CAPLUS, WPIDS, USPATFULL' ENTERED AT 16:07:29 ON 26 JAN 2007

L4 95 S L3  
L5 1 S L4 AND "CELL PROLIFERATION"  
L6 0 S L4 AND "DIFFERENTIATION"  
L7 5 S L4 AND "TUMOR"

=> s l4 and cancer

L8 3 L4 AND CANCER

=> d l8 1-3 ibib, abs, hitstr

'HITSTR' IS NOT A VALID FORMAT FOR FILE 'MEDLINE'

ENTER DISPLAY FORMAT (BIB):ibib, abs

L8 ANSWER 1 OF 3 MEDLINE on STN

ACCESSION NUMBER: 2006351356 MEDLINE Full-text

DOCUMENT NUMBER: PubMed ID: 16766262

TITLE: Attenuation of LDH-A expression uncovers a link between glycolysis, mitochondrial physiology, and tumor maintenance.

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DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)

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DOCUMENT NUMBER: PubMed ID: 12150823

TITLE: A novel mitochondriotoxic small molecule that selectively inhibits tumor cell growth.

AUTHOR: Fantin Valeria R; Berardi Marcelo J; Scorrano Luca; Korsmeyer Stanley J; Leder Philip

CORPORATE SOURCE: Department of Genetics, Harvard Medical School, Boston, Massachusetts 02115, USA.

SOURCE: Cancer cell, (2002 Jul) Vol. 2, No. 1, pp. 29-42.

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AUTHOR: Hockenbery David M  
CORPORATE SOURCE: Fred Hutchinson Cancer Research Center, Seattle, Washington 98109, USA.. dhockenb@fhcrc.org  
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L4 95 S L3  
L5 1 S L4 AND "CELL PROLIFERATION"  
L6 0 S L4 AND "DIFFERENTIATION"



L7 5 S L4 AND "TUMOR"  
L8 3 S L4 AND CANCER

=> s 14 and "cell death"

L9 1 L4 AND "CELL DEATH"

=> d 19 ibib, abs

L9 ANSWER 1 OF 1 MEDLINE on STN  
ACCESSION NUMBER: 2004029169 MEDLINE Full-text  
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L5 1 S L4 AND "CELL PROLIFERATION"  
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L7            5 S L4 AND "TUMOR"  
L8            3 S L4 AND CANCER  
L9            1 S L4 AND "CELL DEATH"

=>

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	34.62	206.93
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-0.78	-0.78

STN INTERNATIONAL LOGOFF AT 16:11:33 ON 26 JAN 2007